

# Defect levels induced by double substitution of B and N in 4H-SiC

E. Igumbor<sup>a,b,\*</sup>, H. T. Danga<sup>a</sup>, E. Omotoso<sup>a</sup>, W. E. Meyer<sup>a,\*\*</sup>

<sup>a</sup>*Department of Physics, University of Pretoria, Pretoria 0002, South Africa.*

<sup>b</sup>*School of Interdisciplinary Research and Graduate Studies, University of South Africa,  
UNISA 0003, Preller Street, Pretoria, South Africa*

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## Abstract

Studies of substitutional impurities in 4H-SiC play a major role in identifying the most enhanced defect levels induced. N and B substitution in 4H-SiC on separate studies reveal that the N<sub>Si</sub> induced negative-U charge state ordering while the B<sub>Si</sub> induced shallow acceptor level. In this report, in order to predict the most stable defect and its electrically active defect levels, the Heyd, Scuseria and Ernzerhof (HSE06) hybrid functional was used to model and predict the energetics and defect levels induced by double substitution of B and N pair (N<sub>Si</sub>B<sub>C</sub>, N<sub>C</sub>B<sub>C</sub>, N<sub>Si</sub>B<sub>Si</sub> and N<sub>C</sub>B<sub>Si</sub>) in a 4H-SiC. While both B and N substituted for C under equilibrium conditions is the most energetically favourable pair, the N and B both substituted for Si has a relatively high formation energy. The energies of the various configurations suggest that the substitution of B and N pair in 4H-SiC is always stable, and the N<sub>C</sub>B<sub>C</sub> is the most energetically favourable defect. While all the defects studied induced

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\*Corresponding author

\*\*Corresponding author

*Email addresses:* [elgumuk@gmail.com](mailto:elgumuk@gmail.com) (E. Igumbor), [wmeyer@up.ac.za](mailto:wmeyer@up.ac.za) ( W. E. Meyer )

acceptor levels, only the  $N_C B_C$  and  $N_{Si} B_C$  induced shallow donor levels. The  $(0/-1)$  acceptor level induced by the defects is close to the conduction band minimum for the case of  $N_C B_C$  and  $N_C B_{Si}$  and deep lying middle of the band gap of  $4H$ -SiC for the  $N_{Si} B_{Si}$  and  $N_{Si} B_C$ .

*Keywords:* Defect, formation energy, charge state, substitution

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## 1. Introduction

Interesting properties of silicon carbide (SiC) are its common unique polytypes ( $2C$ ,  $3C$ ,  $4H$ ,  $6H$ ) and ability to crystallise in many different phases such as cubic, hexagonal and rhombohedral. SiC is a good example of covalent material in which the Si and C atoms are  $sp^3$  hybridized. The different polytypes of SiC differ only in the stacking order which affects mainly their electronic and optical properties [1, 2]. Earlier reports have shown that all polytypes are inert, hard and have high thermal conductivity [1, 2, 3, 4]. Amongst the common polytypes of SiC, the  $4H$  polytype is outstanding. The  $4H$ -SiC is technologically important because it has a large band gap of 3.26 eV at 300 K, a high breakdown electric field device blocking rating, high carrier mobility and high thermal conductivity. All these interesting properties makes  $4H$ -SiC a good material for application where higher blocking voltage and higher temperature are required [5]. For optimal performances of a semiconductor material, a detailed knowledge of point defects present and the understanding of how to control them is essential [5, 6, 7, 8]. Defects in a  $4H$ -SiC are likely to be introduced during crystal growth, and generated in high concentration by ion-implantation. Such defects may be intrinsic or extrinsic, for which the latter contain atoms of a species different to that of the host

crystal. Double substitution of B and N pair in a hexagonal  $4H$ -SiC is a good example of an extrinsic defect. During ion-implantations, defects that are introduced in a material may be annealed using well known techniques such as Deep level transient spectroscopy (DLTS). For example vacancy, substitution and interstitials defects in  $4H$ -SiC have been studied using DLTS technique, ion beam modification, ion-bombardment and electron beam exposure methods [1, 3, 9, 10, 11]. A good number of these defects studied with aforementioned techniques may occur in the form of clusters, defect-complexes antisites, multivacancies and interstitials [12, 13, 14, 15, 16, 17]. Furthermore, the effect of C and B co-implantation as a ratio of implanted C and B ions in SiC, has been reported [9]. The B is a candidate of deep centre in SiC as reported in a photoluminescence measurements (PL) [18]. The DLTS technique and capacitance method results according to Refs [3, 4], reveal the presence of a deep and a shallow B acceptor level in  $6H$ -SiC. Furthermore, B implantation is one of the established methods to produce a  $p$ -type doping SiC substrates, which most times is associated with the creation of undesired radiation damage. This radiation damage by implantation could induce electrically active defect levels in the form of acceptor which may be annealed out at high temperature. A number of studies have been recently reported on the defects produced as a result of ion-implantation [10, 11, 19, 20]. Reports on DLTS and ion-implantation results of  $n$ - and  $p$ -type double implantation and doping in  $4H$ -SiC are already available in literature [21, 21, 22], however, no detailed theoretical study of double substitution of B and N pair ( $n$ - and  $p$ -type doping) in  $4H$ -SiC has been reported. Consequently, we are contributing to the existing knowledge, by providing a theoretical insight

into the defect levels induced by double substitution of the B and N pair in a hexagonal  $4H$ -SiC.

By using a density functional theory with Heyd, Scuseria and Ernzerhof (HSE06) [23] hybrid functional, we show that the different configurations of double substitution of B and N pair in hexagonal  $4H$ -SiC under equilibrium condition are stable and energetically favourable with binding energies within the range of 1.90 to 3.34 eV . Furthermore, we explored the electronic and thermodynamic charge states transition energies of these defects. We predicted that the double substitution of B and N in hexagonal  $4H$ -SiC behaves as a  $p$ -type material as a result of high electronic states populated close to the valence band maximum (VBM). The double substitution of B and N in hexagonal  $4H$ -SiC induced, depending on the lattice sites, shallow or deep defect levels.

## 2. Computational details

Density function theory calculations of double substitution of B and N pair in  $4H$ -SiC were performed using the Vienna *ab-initio* Simulation Package (VASP) [24]. For the B, N, Si and C atoms, the outer valence electrons were treated with the aid of the projector-augmented wave method [25]. The HSE06 with generalised gradient approximation (GGA) functional of Perdew, Burke and Ernzerhof (PBE) [26] were use as exchange correlation functional. This method yields accurate lattice constant  $a$ ,  $c$  and  $c/a$  of 3.07 Å , 10.05 Å and 3.27, respectively, which are in agreement with experimental and theoretical results [27, 28]. According to the HSE06 method, the PBE is mixed with the non-local Fock. For the calculations presented

in this report, a mixing parameter of 25% of the HSE06 was sufficient to predict a band gap of 3.23 eV, which is close to the experiment band gap of 3.26 eV at 300 K [27]. In order to modelled a defect in semiconductor using the supercell approach, it is required to build a supercell from a primitive hexagonal  $4H$ -SiC unit cell. The hexagonal  $4H$ -SiC unit was relaxed with an energy cut-off of 800 eV and the Brillouin zone was integrated with a special Monkhost-Pack k-points of  $8 \times 8 \times 8$ . The forces acting on the atoms were relaxed until it was less than  $0.01 \text{ eV}/\text{\AA}$ . Furthermore, a 96 atoms supercell was constructed from the unit cell and impurity atoms (N and B) were introduced either on the C or Si lattice positions or on both C and Si lattices, depending on the nomenclature of the defect. The choice of the 96 atoms supercell for the defect modelling was adopted after series of supercell convergence for the  $N_C B_C$  were performed using the 72-atoms, 96-atoms, 144-atoms, 288-atoms and 576-atoms supercells. The  $N_C B_C$  modelled using the 96 atoms supercell has the lowest formation energy of 1.31 eV compared to the 72-atoms, 144-atoms, 288-atoms and 576-atoms supercells. For double substitution of the B and N pair in  $4H$ -SiC calculations, the 96 atoms supercell volume was held fixed while all atoms were relaxed until the forces acting on them were less than  $0.01 \text{ eV}/\text{\AA}$ . This was achieved with a convergence criteria of 400 eV for the energy cut-off and a total minimum energy difference lower than  $10^{-5} \text{ eV}$ . The Monkhost-Pack special k-points of  $2 \times 2 \times 2$  was used to integrate the Brillouin zone. For the defect calculation, the formation energy  $E^F = E^F(\text{double} - \text{substitution}, q)$  of the double substitution of the B and N pair in a  $4H$ -SiC as a function of electron Fermi energy ( $\varepsilon_F$ ) in its charge state  $q$  is given as

$$\begin{aligned}
E^F(\text{double} - \text{substitution}, q) &= E(\text{double} - \text{substitution}, q) - E(4H - SiC) \\
&+ \sum_i \Delta(n)_i \mu_i + q[E_{VBM} + \varepsilon_F] + E_{FNV}^q,
\end{aligned}
\tag{1}$$

where the total energy of the double-substitution, total energy of the pristine supercell of 4H-SiC, number of removed or added constituent atoms of type *ith* and the energy of the valence band maximum (VBM) are represented by  $E(\text{double} - \text{substitution}, q)$ ,  $E(4H - SiC)$ ,  $\Delta(n)_i$  and  $E_{VBM}$ , respectively. The correction term  $E_{FNV}^q$  according to the method proposed by Ref. [29] was included to account for the errors that may arise as a result of finite-size effect and defect-defect interactions. The  $\mu_i$  is the chemical potential of the type *ith* constituent atom. The criteria for calculating the chemical potential for the B, N, C and Si atoms and their values were taken from Ref. [30]. The thermodynamic charge state transition level ( $\varepsilon(q/q')$ ) for charge state  $q$  and  $q'$  was calculated as

$$\varepsilon(q/q') = \frac{E(Q) - E(Q')}{q' - q},
\tag{2}$$

where  $E(Q) = E^F(\text{double} - \text{substitution}, q; \varepsilon_F = 0)$  and  $E(Q') = E^F(\text{double} - \text{substitution}, q'; \varepsilon_F = 0)$ .

### 3. Results and Discussion

#### 3.1. Structural and electronic properties

The geometric structure of 4H-SiC supercell shows that the relaxed Si-C bond distance is 1.89 Å, which is in agreement with previous results [30, 31].

Fig. 1 displays the geometric structures of the pristine supercell containing 96 atoms of  $4H$ -SiC (Fig. 1a), the relaxed structure of the  $N_C B_C$  (Fig. 1b) and that of the  $N_{Si} B_C$  (Fig. 1c). The relaxed bond length of the B–Si, N-Si and B-N nearest neighbour for the  $N_C B_C$  are 1.88, 1.87 and 3.09 Å, respectively, while for the  $N_{Si} B_{Si}$  the B-C, N-C and N-B relaxed bond distance are 1.71, 1.64 and 3.08 Å, respectively. These bond lengths are 18% (B-C) and 25% (N-C) less than the S-C bond length. Whereas for the  $N_C B_{Si}$ , the relaxed bond length of the N-Si, B-C and N-B are 1.81, 1.65 and 2.33 Å, respectively. For the  $N_{Si} B_C$ , the 2.9, 2.80 and 2.33 Å are the respective bond length of the N-C, B-Si and N-B. From the results of the relaxed geometric structures, with the exception of the  $N_{Si} B_{Si}$ , we observed that for all defects configuration the bond lengths of the N-Si is smaller than that of the N-C. While with the exception of the  $N_C B_C$ , the bond length of B-C atoms is relatively smaller than the bond length of the B-Si. The difference in bond length which is attributed to the size of the impurity atoms and the host, could play a vital role in determining the energy of formation since a system that experienced more strain is likely to form with a relatively higher formation energy than a system that experienced less strain in the bond length by the participating atoms.

To explore the activities of impurities in  $4H$ -SiC, we reported the results of the electronic properties for different configurations of double substitution of the B and N pair in  $4H$ -SiC. Fig. 2 displays the plots of the total density of state (TDOS) on the left of each plot and the partial density of state (PDOS) on the right of each plot. For the  $N_C B_C$  as shown in Fig. 2a, the DOS plot reveals that the electronic states are mainly populated at the VBM.

The  $2p$ -orbital of B atom is a major contributor of the states lying close to the Fermi level. Furthermore, couple of strong orbital hybridization by the participating atomic orbitals was observed in all the defects. This strong hybridization of the orbitals is from the  $2p$ -orbital of the C, N and B atoms. For the  $N_C B_C$ , the valence electron orbitals of Si which is less present, is close to the VBM. All the defects investigated in this report have their ground state electron thickly populated at the VBM close to the Fermi level. This suggests that the double substitution of B and N exhibit the properties of a  $p$ -type material. Whereas the  $N_C B_C$  and  $N_{Si} B_C$  have sharp peak almost at the Fermi level which were contributed by the  $p$ -orbital of B atom, the  $N_{Si} B_{Si}$  and  $N_C B_{Si}$  on the other hand did not shown any sign of sharp peak close to the Fermi level. In addition, for all the defect considered, strong orbital hybridization between the B- $2p$ , N- $2p$  and C- $2p$  orbitals were observed mainly at the VBM. This suggest that these impurities in  $4H$ -SiC behave as  $p$ -type materials with excess electron at the VBM. The TDOS plots reveal that inspite of the external impurities introduced into  $4H$ -SiC, the system still retains its wide band gap nature.

### *3.2. Formation energy and defect transition level*

For us to ascertained the stability of the  $N_C B_C$ ,  $N_C B_{Si}$ ,  $N_{Si} B_{Si}$  and  $N_{Si} B_C$ , we calculated their formation and binding energies. Table 1 displays the energy of formation and binding energies of the substitution of N and B pair in  $4H$ -SiC. These energies were calculated under chemical rich conditions. The formation energy for the neutral charge state of the  $N_{Si} B_C$ ,  $N_{Si} B_{Si}$ ,  $N_C B_C$  and  $N_C B_{Si}$  are 1.37, 9.86, 1.31 and 1.37 eV, respectively. The result of the formation energies show that for the neutral charge state, the  $N_C B_C$  and



$N_C B_{Si}$  are energetically more stable than the  $N_{Si} B_{Si}$  and  $N_{Si} B_C$ . This scenario suggests that the substitution of the B and N pair in  $4H$ -SiC prefer to be substituted on the C lattice sites as against Si lattice sites with relatively lower formation energy. Furthermore, the results of the formation energy suggests that  $N_C B_C$  and  $N_C B_{Si}$  defects can be accomplished experimentally at a relatively low energy compared to the synthesis of  $N_{Si} B_{Si}$  and  $N_C B_C$  defects. The relatively higher energy of the  $N_{Si} B_{Si}$  and  $N_{Si} B_C$  compared to the  $N_C B_C$  and  $N_C B_{Si}$  can be attributed to the the higher formation energy of the  $N_{Si}$  compare to the  $N_C$ . Reports have suggested that the formation energy of the  $N_C$  is always lower than that of the  $N_{Si}$  [32]

Before charges are introduced into defect-complex system such as double substitution pair, it is always important to check the stability of the defect-complex. This is usually checked by calculating the binding energy as [8, 33]

$$E_b = \Sigma E^F(X_i) - E^F(\text{double} - \text{substituion}), \quad (3)$$

where  $E^F(X_i)$  and  $E^F(\text{double} - \text{substituion})$  are the formation energies of a type *ith* substitution and double substitution of B and N pair in  $4H$ -SiC, respectively. By using Eq. 3, we obtained the binding energies of the  $N_C B_C$ ,  $N_C B_{Si}$ ,  $N_{Si} B_{Si}$  and  $N_{Si} B_C$  as displayed by Table 1. All the binding energies are positive suggesting that the double substitutions of B and N in  $4H$ -SiC are always stable. This further shows that these defects under study can only dissociate into smaller fragments of non-interacting defects at the expense of a high energy of formation. In addition, we observed that the  $N_{Si} B_C$  even with a relatively high energy of formation compared to the  $N_C B_C$ ,  $N_C B_{Si}$ , has a relatively higher binding energy. This corroborate that much energy

is needed to split this defect compare to other defects and also show that in an environment where high power, high frequency devices are needed,  $N_{Si}B_C$  could be a possible candidate. As expected the  $N_C B_{Si}$  with comparably low formation energy of 1.37 eV has a binding energy of 3.31 eV. Our results have shown that different impurities at Si lattice sites are always less stable than when the atoms are on the C lattice sites.

Fig. 3 shows the formation energy as a function of the Fermi energy for the double substitution of B and N pair in  $4H$ -SiC. Table 2 displays the charge state transition ( $\varepsilon(q/q')$ ) levels above the VBM in eV induced by the substitution of B and N pair in  $4H$ -SiC. The  $N_C B_C$  induced two distinct defect levels, the  $(+1/0)$  and  $(0/-1)$  as shown in Fig. 3a. For the  $(+1/0)$  single donor level, the energy is lying shallow at 0.28 eV far away from the VBM, while the shallow acceptor level  $(0/-1)$  energy is  $E_C - 0.20$  eV. The  $N_{Si} B_{Si}$  induced double acceptor levels (see Fig. 3b), the  $(0/-1)$  and  $(-1/-2)$  which have energies of  $E_V + 0.1.85$  and  $E_V + 2.32$  eV, respectively. While the  $N_C B_{Si}$  induced a single defect level in the band gap of  $4H$ -SiC (as shown in Fig. 3c), the  $N_{Si} B_C$  induced three distinct defect levels displayed in Fig. 3d. For the  $N_C B_{Si}$ , the  $(0/-1)$  acceptor level is shallow lying at  $E_C - 0.16$  eV. The  $N_{Si} B_C$  defect levels are shallow donor  $(+1/0)$  with energy of  $E_V + 0.08$  eV, and deep acceptors  $(0/-1)$  and  $(-1/-2)$  with energies of  $E_V + 2.30$  and  $E_V + 2.75$  eV, respectively. A critical examination of the defects reveal that the double substitution of the B and N pair in  $4H$ -SiC does not induced double donor level. However, the defects in its unique configuration induced shallow donor levels (for the pair with  $B_C$ ) and deep acceptor levels (for the pair with  $N_{Si}$ ).

## 4. Summary

The results of double substitution of N and B impurities pair in 4H-SiC were modelled within the framework of density functional theory (DFT). Our results show that double substitution of N and B in 4H-SiC are energetically stable with respect to their binding energies. The  $N_C B_C$  and  $N_C B_{Si}$  are energetically most favourable under equilibrium conditions. Defect levels induced by the N and B double substitution in 4H-SiC are shallow for single donor and deep for the double acceptor level. Whereas the  $N_C B_C$  induced defect levels are always shallow, the  $N_{Si} B_{Si}$  induced acceptor levels are always deep. The  $N_{Si} B_C$  shallow donor level is 0.08 eV far away from the valence band maximum. These results provide a theoretical insight for future work which is crucial for improving the quality of SiC devices.

## 5. Acknowledgement

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Table 1: The energy of formation ( $E^F$ ) and binding energy ( $E_B$ ) in eV at  $\varepsilon_F=0$  for the substitution of N and B pair in 4H-SiC. The  $E^F$  and  $E_B$  energies were calculated under chemical potential rich conditions.

	$N_C B_C$	$N_{Si} B_{Si}$	$N_C B_{Si}$	$N_{Si} B_C$
$E^F$	1.31	9.86	1.37	7.96
$E_B$	2.91	1.90	3.31	3.34

Table 2: The charge state transition ( $\varepsilon(q/q')$ ) levels above the VBM in eV induced by the substitution of B and N pair in 4H-SiC.

Defect	(+1/0)	(0/ - 1)	(-1/ - 2)
$N_C B_C$	0.28	3.13	—
$N_{Si} B_{Si}$	—	1.85	2.32
$N_C B_{Si}$	—	3.07	—
$N_{Si} B_C$	0.08	2.30	2.75



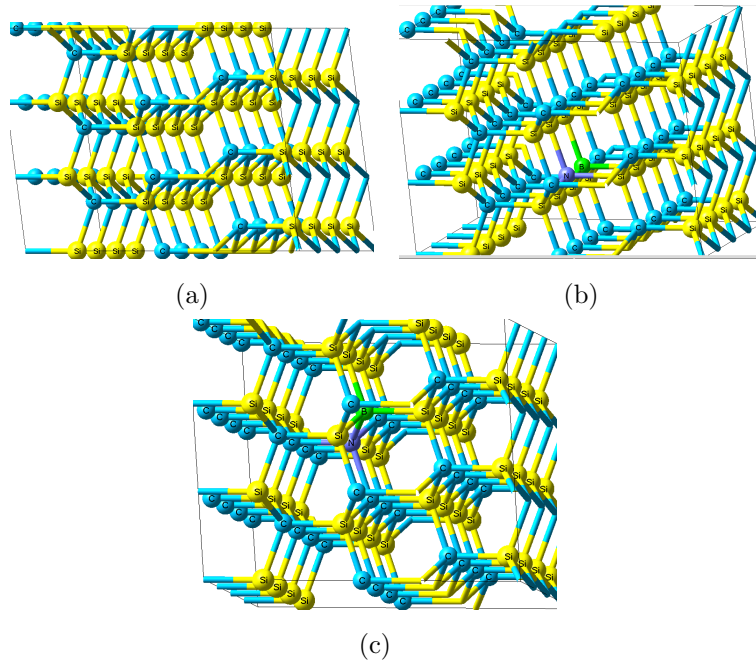


Figure 1: Relaxed geometric structures of (a) 96 atoms supercell of  $4H$ -SiC (b) supercell containing the N and B atoms sitting at the lattice sites of C in  $4H$ -SiC ( $N_C B_C$ ) and (c) supercell containing the N and B atoms, respectively sitting at the lattice sites of Si and C in  $4H$ -SiC ( $N_{Si} B_C$ ).

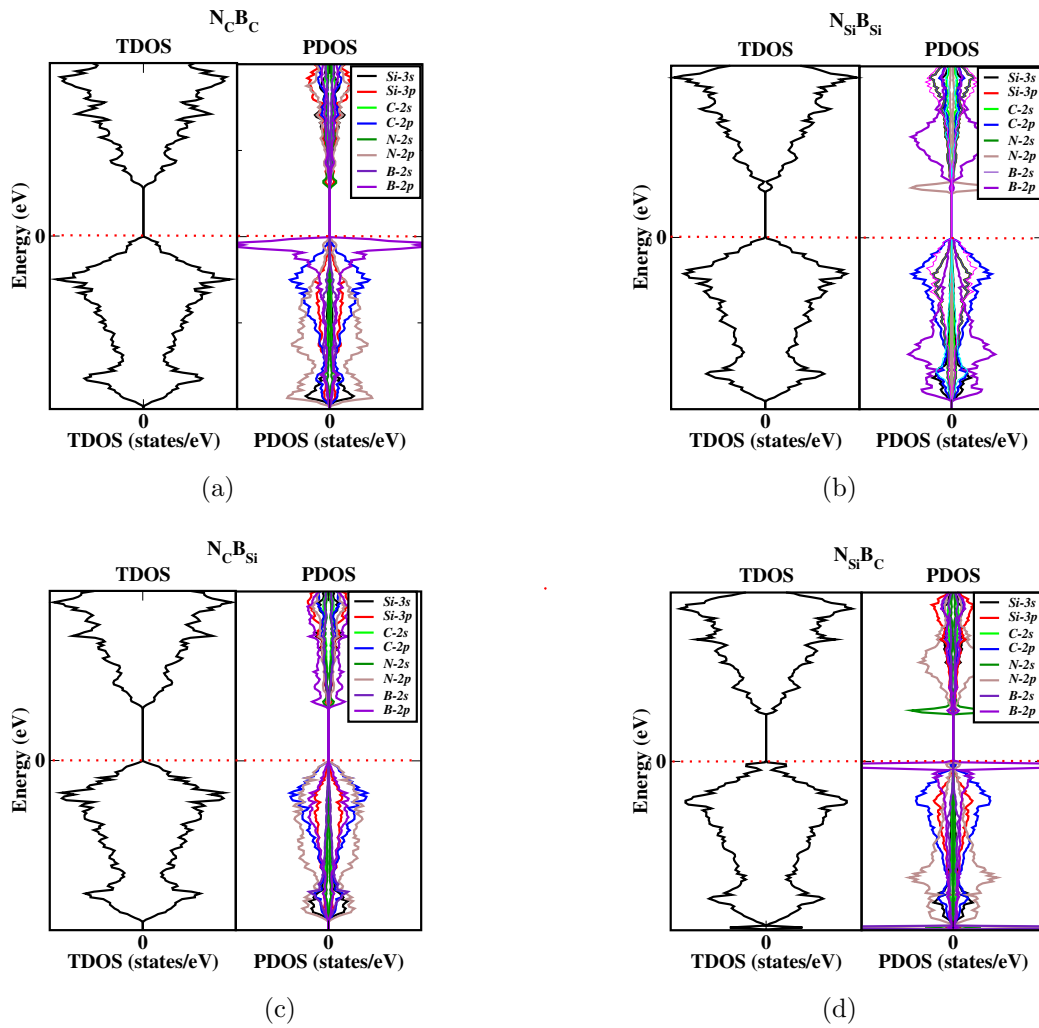


Figure 2: Plot of the total density of states (TDOS) and partial density of states (PDOS) for the (a)  $N_C B_C$ ; (b)  $N_{Si} B_{Si}$ ; (c)  $N_C B_{Si}$  and (d)  $N_{Si} B_C$ . The horizontal dashed line is the Fermi level, which is set to zero ( $\varepsilon_F=0$ ).

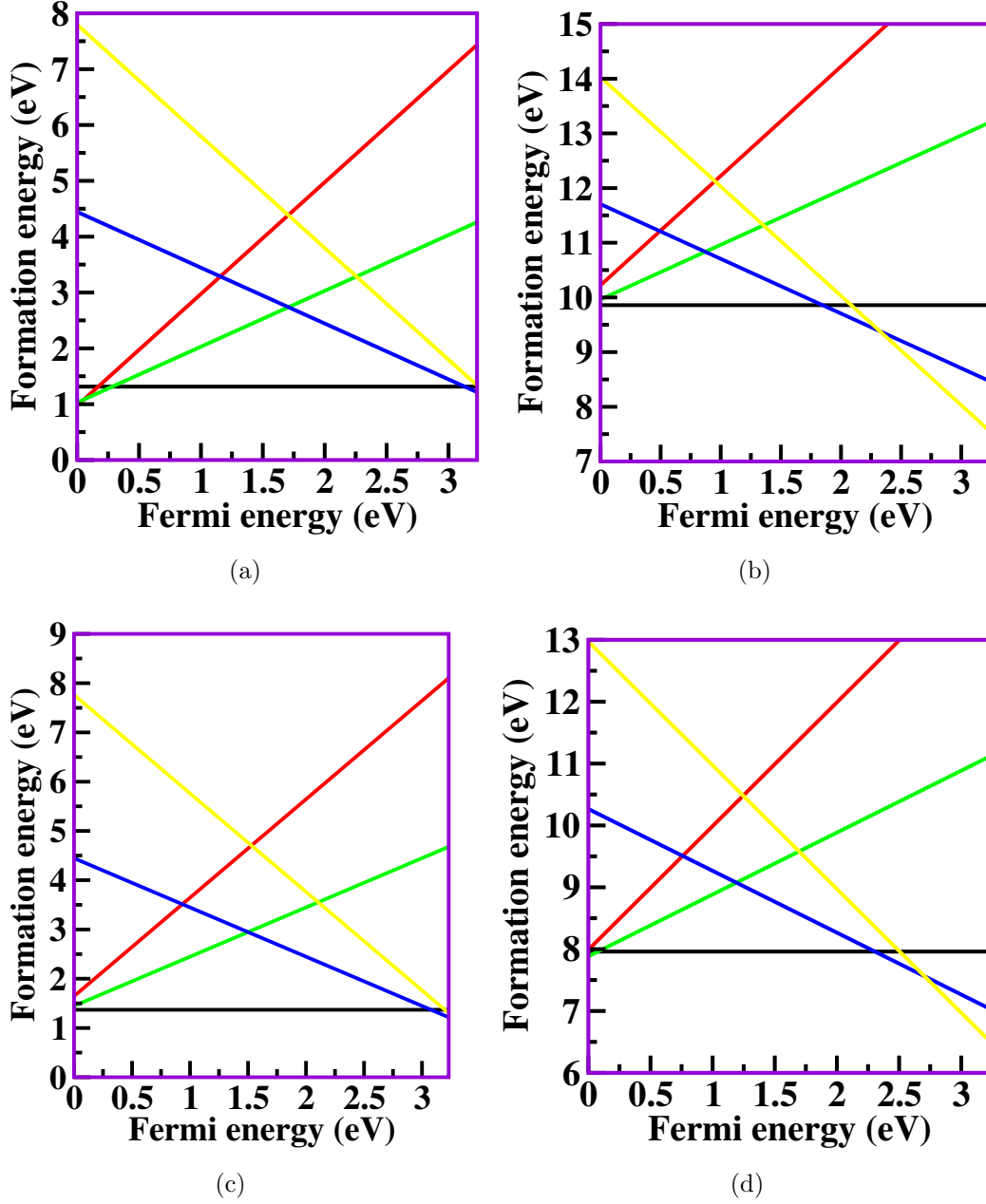


Figure 3: Plot of formation energy as a function of the Fermi energy for the substitution of the B and N pair in 4H-SiC, (a)  $N_C B_C$ , (b)  $N_{Si} B_{Si}$ , (c)  $N_C B_{Si}$  and (d)  $N_{Si} B_C$ . The slope of each graph corresponds to the charge state as defined in Eq. 2.